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TRAC METHODS AND MODELS

by

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ABSTRACT

The numerical methods and physical models used in the Transient Reactor Analysis Code (TRAC) versions PD2 and PF1 are discussed. Particular emphasis is placed on TRAC-PF1, the version specifically designed to analyze small-break loss-of-coolant accidents (LOCAs).

I. INTRODUCTION

The Transient Reactor Analysis Code (TRAC) was originally chartered as an advanced best-estimate code for large-break LOCA analysis of pressurized water reactors (PWRs). However, during the development of TRAC-PD2,¹ attention was shifted to small-break LOCAs by the accident at Three Mile Island (TMI). Minor modifications were made to PD2 to allow reasonably efficient and accurate calculations of small-break accidents, but TRAC-PF1 was designed specifically as a high-performance, best-estimate code for analyzing these events.

Most TRAC-PD2 development involved improving the calculation of reflood beyond the capability available in TRAC-PIA.² The largest single change was the addition of two-dimensional rod heat conduction with automatic fine-mesh rezoning for accurate tracking of the quench front. The method was similar to one already in use in COBRA.³ An inverted annular flow regime and subcooled boiling model were added to the code, and several minor changes made to improve the behavior of the numerics during refill and reflood. When the first attempts were made with this code to perform analyses of TMI system damage, significant numerical mass conservation errors were discovered. These were corrected by improving the matrix solution procedures in the vessel component. Beyond this, no significant changes were required to allow PD2 to model this class of small-break LOCAs.

TRAC-PF1 was created to correct a number of limitations in PD2. The first was the time step restriction of the material Courant stability limit (time step less than mesh length divided by material velocity). Although PD2 could exceed this limit within fully implicit components, the limit was still in force in semi-implicit components and at all component junctions. In small-break accidents the time step size required by this limit is almost always far smaller than the size required for reasonable accuracy if stability is not a problem. In TRAC-PF1 a stability-enhancing two-step (SETS) method^{4,5} is used to eliminate the material Courant limit from all regions of a reactor modeled in one dimension. The computational cost per cell per time step for SETS is only one-fifth that of standard fully implicit techniques and only 20% more than the semi-implicit method. To take full advantage of this new numerical capability, a one-dimensional core component was added to PF1 to allow modeling of an entire reactor system in one dimension. The three-dimensional vessel also was retained so that PF1 contains all the modeling features of PD2. Another limitation of PD2 was the use of a drift-flux formulation for the flow equations in one-dimensional components. This form of the equations does not adapt well to the modeling of either counter-current or stratified flow. In PF1, the two-fluid model that was previously only available in the three-dimensional vessel model has been extended to the one-dimensional components, permitting accurate calculations of counter-current flow and the addition of a stratified-flow regime. Other important features in PF1 are an additional field to allow for the tracking of noncondensable gas, reactivity feedback, and significantly improved trip and control logic.

In the following sections details of the methods and models used in TRAC-PF1 are described. Comments are made where appropriate on the differences from PD2.

II. FLOW EQUATIONS

Unlike TRAC versions preceding TRAC-PF1, the same two-phase two-fluid model for fluid flow is used now in both one- and three-dimensional components. In addition, a noncondensable gas component has been included in the vapor field, requiring one extra mass continuity equation. Homogeneity and thermal equilibrium are assumed for the combined gas field.

The seven differential equations describing the three-component, two-fluid model are:

Liquid Mass Equation

$$\frac{\partial(1 - \alpha)\rho_l}{\partial t} + \nabla \cdot [(1 - \alpha)\rho_l \vec{V}_l] = -\Gamma, \quad (1)$$

Combined Vapor Mass Equation

$$\frac{\partial(\alpha\rho_g)}{\partial t} + \nabla \cdot (\alpha\rho_g \vec{V}_g) = \Gamma, \quad (2)$$

Noncondensable Gas Mass Equation

$$\frac{\partial(\alpha\rho_a)}{\partial t} + \nabla \cdot (\alpha\rho_a \vec{V}_g) = 0, \quad (3)$$

Combined Vapor Equation of Motion

$$\begin{aligned} \frac{\partial \vec{V}_g}{\partial t} + \vec{V}_g \cdot \nabla \vec{V}_g = & -\frac{c_l}{\alpha\rho_g} (\vec{V}_g - \vec{V}_l) |\vec{V}_g - \vec{V}_l| - \frac{1}{\rho_g} \nabla p \\ & - \frac{c_{wg}}{\alpha'\rho_g} \vec{V}_g |\vec{V}_g| + \vec{g}, \end{aligned} \quad (4)$$

Liquid Equation of Motion

$$\begin{aligned} \frac{\partial \vec{v}_\ell}{\partial t} + \vec{v}_\ell \cdot \nabla \vec{v}_\ell &= \frac{c_1}{(1-\alpha)\rho_\ell} (\vec{v}_g - \vec{v}_\ell) |\vec{v}_g - \vec{v}_\ell| - \frac{1}{\rho_\ell} \nabla p \\ &- \frac{c_{w\ell}}{(1-\alpha)\rho_\ell} \vec{v}_\ell |\vec{v}_\ell| + \vec{g} \quad , \end{aligned} \quad (5)$$

Combined Vapor Energy Equation

$$\begin{aligned} \frac{\partial}{\partial t} (\alpha \rho_g e_g) + \nabla \cdot (\alpha \rho_g e_g \vec{v}_g) \\ = - p \frac{\partial \alpha}{\partial t} - p \nabla \cdot (\alpha \vec{v}_g) + q_{wg} + q_{lg} + \Gamma h_{sg} \quad , \end{aligned} \quad (6)$$

and the Total Energy Equation

$$\begin{aligned} \frac{\partial [(1-\alpha)\rho_\ell e_\ell + \alpha\rho_g e_g]}{\partial t} + \nabla \cdot [(1-\alpha)\rho_\ell e_\ell \vec{v}_\ell + \alpha\rho_g e_g \vec{v}_g] \\ = - p \nabla \cdot [(1-\alpha)\vec{v}_\ell + \alpha\vec{v}_g] + q_{w\ell} + q_{wg} \quad . \end{aligned} \quad (7)$$

In these equations the vapor densities and energies are sums of the steam and noncondensable components

$$\rho_g = \rho_s + \rho_a \quad (8)$$

$$\rho_g e_g = \rho_s e_s + \rho_a e_a \quad . \quad (9)$$

Currently, Dalton's law is assumed to hold so that

$$p = p_s + p_a \quad . \quad (10)$$

A subscript of a is used for the noncondensable gas because it is used primarily to model air. This default can be overridden with input to use the field for tracking hydrogen in severe accidents.

In addition to the thermodynamic relations that are required for closure, specifications for the interfacial drag coefficients (c_i), the interfacial heat transfer (q_{ig}), the phase-change rate (Γ), the wall shear coefficients (C_{wg} and C_{wl}), and the wall heat transfers (q_{wg} and q_{wl}) are required. Gamma is evaluated from a simple thermal energy jump relation,

$$\Gamma = \frac{-q_{ig} - q_{il}}{h_{sg} - h_{sl}}, \quad (11)$$

where

$$q_{ig} = h_{ig} A_i \frac{(T_{ss} - T_g)}{vol} \quad (12)$$

and

$$q_{il} = h_{il} A_i \frac{(T_{ss} - T_l)}{vol} . \quad (13)$$

Here A_i and the h_i 's are the interfacial area and heat transfer coefficients, and T_{ss} is the saturation temperature corresponding to the partial pressure of steam.

Wall heat-transfer terms assume the form

$$q_{wg} = h_{wg} A_{wg} \frac{T_w - T_g}{vol} \quad (14)$$

and

$$q_{wl} = h_{wl} A_{wl} \frac{T_w - T_l}{vol} , \quad (15)$$

where A_{wg} and A_{wl} are the actual heated surface areas of the cell, except during reflood when the average heat-transfer coefficients reflect the fraction of the heated surface area that is quenched.

III. ONE-DIMENSIONAL FINITE-DIFFERENCE METHODS

In TRAC-PF1 the spacial differencing in the one-dimensional components is the same as that used in the three-dimensional vessel; however, a new approach to time integration has been applied. As previously indicated, the SETS method eliminates the material Courant stability limit from all one-dimensional components. That limit now only applies in vessels and at junctions between vessels and one-dimensional components. Because the finite-difference method used in the vessel is documented thoroughly elsewhere,^{1,2} we will only discuss the SETS difference equations here.

The stability-enhancing two-step method consists of a basic step (that is almost identical to the standard semi-implicit methods used in the vessel) and a stabilizing step. For homogeneous flow, the ordering of these steps does not matter. However, for two-fluid flow with noticeable relative velocity it is necessary to do the stabilizing step for the equations of motion before the basic step. When this stabilizing step precedes the basic step, an initial explicit prediction of velocities gives strong coupling through the interfacial drag terms without requiring direct communication between the stabilizing equations for liquid and vapor motion. To provide improved conservation and to minimize machine storage required in TRAC, the stabilizing steps for mass and energy equations are done as the final portion of the calculation.

The spacial mesh used for the finite-difference equations is staggered with thermodynamic properties evaluated at the cell centers and velocities evaluated at the cell edges. For stability, flux terms at cell edges require donor cell averages of the form

$$\begin{aligned} \langle YV \rangle_{j+1/2} &= Y_j V_{j+1/2}, V_{j+1/2} \geq 0 \\ &= Y_{j+1} V_{j+1/2}, V_{j+1/2} < 0 \end{aligned} \quad (16)$$

where Y can be any cell-center state variable or combination of such variables and V may be either liquid or vapor velocity. With this notation the finite-difference divergence operator for one-dimensional calculations is

$$V_j \cdot (YV) = (A_{j+1/2} \langle YV \rangle_{j+1/2} - A_{j-1/2} \langle YV \rangle_{j-1/2}) / \text{vol}_j \quad (17)$$

where A is the local cross-sectional area and vol_j is the volume of the j th cell. For the equations of motion the donor cell form of any VVV term is

$$\begin{aligned}
 & v_{j+1/2} (v_{j+1/2} - v_{j-1/2}) / \Delta x_{j+1/2}, \quad v_{j+1/2} \geq 0 \\
 & v_{j+1/2} \nabla_{j+1/2} v = \\
 & v_{j+1/2} (v_{j+3/2} - v_{j+1/2}) / \Delta x_{j+1/2}, \quad v_{j+1/2} < 0,
 \end{aligned} \tag{18}$$

where $\Delta x_{j+1/2}$ is half the sum of Δx_j and Δx_{j+1} .

The finite-difference equations currently used (roughly in order of their calculation) are:

Predictor for Equations of Motion

$$\begin{aligned}
 & (\hat{v}_g^{n+1} - v_g^n) / \Delta t + v_g^n \nabla_{j+1/2} \tilde{v}_g^n + \beta (\hat{v}_g^{n+1} - v_g^n) \nabla_{j+1/2} \tilde{v}_g^n \\
 & + \frac{C_1^n}{(\bar{\alpha}\bar{\rho}_g)_{j+1/2}^n} (2(\hat{v}_g^{n+1} - \hat{v}_\ell^{n+1}) - (v_g^n - v_\ell^n)) |v_g^n - v_\ell^n| \\
 & + \frac{1}{(\bar{\rho}_g)_{j+1/2}^n} (p_{j+1}^n - p_j^n) / \Delta x_{j+1/2} \\
 & + \frac{C_{wg}}{(\bar{\alpha}\bar{\rho}_g)_{j+1/2}^n} (2 \hat{v}_g^{n+1} - v_g^n) |v_g^n| + g \cos \theta = 0,
 \end{aligned} \tag{19}$$

where

$$0, \quad \nabla_{j+1/2} v^n \leq 0$$

$\beta =$

$$1, \quad \nabla_{j+1/2} v^n > 0,$$

$$(\hat{v}_\ell^{n+1} - v_\ell^n) / \Delta t + v_\ell^n \nabla_{j+1/2} \tilde{v}_\ell^n + \beta (\hat{v}_\ell^{n+1} - v_\ell^n) \nabla_{j+1/2} \tilde{v}_\ell^n$$

$$+ \frac{C_1^n}{[(1-\alpha)\rho_\ell]^n_{j+1/2}} [2(\hat{v}_\ell^{n+1} - \hat{v}_g^{n+1}) - (v_\ell^n - v_g^n)] |v_g^n - v_\ell^n|$$

(20)

$$+ \frac{1}{(\bar{\rho}_\ell)^n_{j+1/2}} (p_{j+1}^n - p_j^n)/\Delta x_{j+1/2}$$

$$+ \frac{C_{w\ell}}{[(1-\alpha)\rho_\ell]^n_{j+1/2}} (2 \hat{v}_\ell^{n+1} - v_\ell^n) |v_\ell^n| + g \cos \theta = 0 \quad ;$$

Stabilizer Equations of Motion

$$(\tilde{v}_g^{n+1} - v_g^n)/\Delta t + v_g^n \nabla_{j+1/2} \tilde{v}_g^{n+1} + \beta(\tilde{v}_g^{n+1} - v_g^n) \nabla_{j+1/2} \tilde{v}_g^n$$

$$+ \frac{C_1^n}{(\bar{\alpha}\rho_g)^n_{j+1/2}} [2(\hat{v}_g^{n+1} - \hat{v}_\ell^{n+1}) - (v_g^n - v_\ell^n)] |v_g^n - v_\ell^n| \quad (21)$$

$$+ \frac{1}{(\bar{\rho}_g)^n_{j+1/2}} (p_{j+1}^n - p_j^n)/\Delta x_{j+1/2}$$

$$+ \frac{C_{wg}}{(\bar{\alpha}\rho_g)^n_{j+1/2}} (2 \tilde{v}_g^{n+1} - v_g^n) |v_g^n| + g \cos \theta = 0 \quad ,$$

$$(\tilde{v}_\ell^{n+1} - v_\ell^n)/\Delta t + v_\ell^n \nabla_{j+1/2} \tilde{v}_\ell^{n+1} + \beta(\tilde{v}_\ell^{n+1} - v_\ell^n) \nabla_{j+1/2} \tilde{v}_\ell^n \quad (22)$$

$$+ \frac{C_1^n}{[(1-\alpha)\rho_\ell]^n_{j+1/2}} [2(\hat{v}_\ell^{n+1} - \hat{v}_g^{n+1}) - (v_\ell^n - v_g^n)] |v_g^n - v_\ell^n|$$

$$\begin{aligned}
 & + \frac{1}{(\bar{\rho}_\ell)^n_{j+1/2}} (p_{j+1}^n - p_j^n) / \Delta x_{j+1/2} \\
 & + \frac{C_{w\ell}}{[(1-\alpha)\bar{\rho}_\ell]^n_{j+1/2}} (2 \tilde{v}_\ell^{n+1} - v_\ell^n) |v_\ell^n| + g \cos \theta = 0 ,
 \end{aligned}$$

Basic Equations of Motion

$$\begin{aligned}
 & (v_g^{n+1} - v_g^n) / \Delta t + v_g^n \nabla_{j+1/2} \tilde{v}_g^{n+1} + \beta (v_g^{n+1} - v_g^n) \nabla_{j+1/2} \tilde{v}_g^n \\
 & + \frac{C_1^n}{(\bar{\alpha}\bar{\rho}_g)^n_{j+1/2}} [2(v_g^{n+1} - v_\ell^{n+1}) - (v_g^n - v_\ell^n)] |v_g^n - v_\ell^n| \quad (23) \\
 & + \frac{1}{(\bar{\rho}_g)^n_{j+1/2}} (\tilde{p}_{j+1}^{n+1} - \tilde{p}_j^{n+1}) / \Delta x_{j+1/2} \\
 & + \frac{C_{wg}}{(\bar{\alpha}\bar{\rho}_g)^n_{j+1/2}} (2 v_g^{n+1} - v_g^n) |v_g^n| + g \cos \theta = 0 ,
 \end{aligned}$$

$$\begin{aligned}
 & (v_\ell^{n+1} - v_\ell^n) / \Delta t + v_\ell^n \nabla_{j+1/2} \tilde{v}_\ell^{n+1} + \beta (v_\ell^{n+1} - v_\ell^n) \nabla_{j+1/2} \tilde{v}_\ell^n \\
 & + \frac{C_1^n}{[(1-\alpha)\bar{\rho}_\ell]^n_{j+1/2}} [2(v_\ell^{n+1} - v_g^{n+1}) - (v_\ell^n - v_g^n)] |v_\ell^n - v_g^n| \\
 & + \frac{1}{(\bar{\rho}_\ell)^n_{j+1/2}} (\tilde{p}_{j+1}^{n+1} - \tilde{p}_j^{n+1}) / \Delta x_{j+1/2} \quad (24) \\
 & + \frac{C_{w\ell}}{[(1-\alpha)\bar{\rho}_\ell]^n_{j+1/2}} (2 v_\ell^{n+1} - v_\ell^n) |v_\ell^n| + g \cos \theta = 0 ;
 \end{aligned}$$

Basic Mass Equations

$$[(\tilde{\alpha}\tilde{\rho}_g)^{n+1} - (\alpha\rho_g)^n]/\Delta t + \nabla_j \cdot (\alpha\rho_g v_g^{n+1}) = \tilde{\Gamma}^{n+1} , \quad (25)$$

$$[(\tilde{\alpha}\tilde{\rho}_a)^{n+1} - (\alpha\rho_a)^n]/\Delta t + \nabla_j \cdot (\alpha\rho_a v_g^{n+1}) = 0 , \quad (26)$$

$$[(1 - \tilde{\alpha})^{n+1} \tilde{\rho}_\ell^{n+1} - (1 - \alpha)^n \rho_\ell^n]/\Delta t + \nabla_j \cdot [(1 - \alpha) \rho_\ell v_\ell^{n+1}] = - \tilde{\Gamma}^{n+1} ; \quad (27)$$

Basic Energy Equations

$$[(\tilde{\alpha}\tilde{\rho}_g \tilde{e}_g)^{n+1} - (\alpha\rho_g e_g)^n]/\Delta t + \nabla_j \cdot (\alpha\rho_g e_g v_g^{n+1}) \quad (28)$$

$$+ \tilde{p}^{n+1} [(\tilde{\alpha}^{n+1} - \alpha^n)/\Delta t + \nabla_j \cdot (\alpha^n v_g^{n+1})]$$

$$= \tilde{q}_{wg}^{n+1} + \tilde{q}_{lg}^{n+1} + \tilde{\Gamma}^{n+1} \tilde{h}_{sg}^{n+1} ,$$

$$\{[\tilde{\alpha}\tilde{\rho}_g \tilde{e}_g + (1 - \tilde{\alpha}) \tilde{\rho}_\ell \tilde{e}_\ell]^{n+1} - [\alpha\rho_g e_g + (1 - \alpha) \rho_\ell e_\ell]^n\}/\Delta t \quad (29)$$

$$+ \nabla_j \cdot [(\alpha\rho_g e_g) v_g^{n+1} + (1 - \alpha) \rho_\ell e_\ell v_\ell^{n+1}]$$

$$+ \tilde{p}^{n+1} \nabla_j \cdot [(1 - \alpha)^n v_\ell^{n+1} + \alpha^n v_v^{n+1}] = \tilde{q}_{wg}^{n+1} + \tilde{q}_{w\ell}^{n+1} ;$$

Stabilizing Mass Equations

$$[(\alpha\rho_g)^{n+1} - (\alpha\rho_g)^n]/\Delta t + \nabla_j \cdot [(\alpha\rho_g)^{n+1} v_g^{n+1}] = \tilde{\Gamma}^{n+1} \quad (30)$$

$$[(\alpha\rho_a)^{n+1} - (\alpha\rho_a)^n]/\Delta t + \nabla_j \cdot [(\alpha\rho_a)^{n+1} v_g^{n+1}] = 0 \quad (31)$$

$$[(1 - \alpha)^{n+1} \rho_\ell^{n+1} - (1 - \alpha)^n \rho_\ell^n] / \Delta t + \nabla_j \cdot [(1 - \alpha)^{n+1} \rho_\ell^{n+1} v_\ell^{n+1}] = - \tilde{\Gamma}^{n+1} ; \quad (32)$$

Stabilizing Energy Equations

$$\begin{aligned} & [(\alpha \rho_g e_g)^{n+1} - (\alpha \rho_g e_g)^n] / \Delta t + \nabla_j \cdot [(\alpha \rho_g e_g)^{n+1} v_g^{n+1}] \\ & + \tilde{p}^{n+1} [(\tilde{\alpha}^{n+1} - \alpha^n) / \Delta t + \nabla_j \cdot (\alpha^n v_g^{n+1})] \\ & = \tilde{q}_{ig}^{n+1} + \tilde{q}_{wg}^{n+1} + \tilde{\Gamma}^{n+1} \tilde{h}_{sg}^{n+1} , \end{aligned} \quad (33)$$

$$\begin{aligned} & \{[(1 - \alpha) \rho_\ell e_\ell]^{n+1} - [(1 - \alpha) \rho_\ell e_\ell]^n\} / \Delta t + \nabla_j \cdot \{[(1 - \alpha) \rho_\ell e_\ell]^{n+1} v_\ell^{n+1}\} \\ & + \tilde{p}^{n+1} \{(\alpha^n - \tilde{\alpha}^{n+1}) / \Delta t + \nabla_j \cdot [(1 - \alpha)^n v_\ell^{n+1}]\} \\ & = \tilde{q}_{w\ell}^{n+1} - \tilde{q}_{ig}^{n+1} - \tilde{\Gamma}^{n+1} \tilde{h}_{sg}^{n+1} . \end{aligned} \quad (34)$$

A caret is used above velocities to denote explicit predictor values. A tilde above a variable indicates that it is the result of an intermediate step and not a final value for the end of the time step. A horizontal line above a quantity indicates that it is obtained with a 50% average between values at adjacent cells. Subscripts denoting cell location that are absent can be assumed to be j for mass and energy equations and $j+1/2$ for equations of motion. Finally, θ is the angle between a vector from the center of cell j to the center of $j+1$ and a vector pointing straight up.

Time levels have been left off parts of the flux terms in Eqs. (25) through (29) because they contain a mixture of old and new time quantities. If X is a combination of state variables without a time superscript, then the correct definition for the divergence term in which it appears is

$$\begin{aligned} \nabla_j (X v_j^{n+1}) &= \{A_{j+1/2} v_{j+1/2}^{n+1} [f_{j+1/2} X_j^m + (1 - f_{j+1/2}) X_{j+1}^n] \\ &- A_{j-1/2} v_{j-1/2}^{n+1} [f_{j-1/2} X_{j-1}^n + (1 - f_{j-1/2}) X_j^m]\} / vol_j , \end{aligned} \quad (35)$$

where

$$x_j^m = g' x_j^n + (1 - g') x_j^{n+1}. \quad (36)$$

f is the weighing function used to obtain donor cell averaging [Eq. (7)], and g' is a weighing factor depending on the rate of phase change that goes to unity as phase change disappears and to zero as the phase change approaches the total outflow of the phase created in the cell. For nonzero g' this form of the divergence operator is nonconservative but total conservation is maintained by the stabilizer step.

Equations (19) and (20) do not involve any implicit coupling between cells and can be solved rapidly for each cell. Because Eqs. (21) and (22) do not couple to each other, each one requires only the solution of a tridiagonal linear system. Equations (23) through (29), combined with the necessary thermodynamic and constitutive equations, form a coupled system of nonlinear equations. Equations (23) and (24) are solved directly to obtain v_g^{n+1} and v_l^{n+1} as dependent variables. After substituting these equations for velocity into Eqs. (25) through (29), the resulting system is solved for the independent variables p^{n+1} , p_a^{n+1} , T_g^{n+1} , T_l^{n+1} , and α^{n+1} with a standard Newton iteration, including all coupling between cells. In practice, the linearized equations solved during this iteration can be reduced easily to a tridiagonal system involving only total pressures. The final five stabilizing equations [(30) through (34)] are also simple tridiagonal linear systems, as v_g^{n+1} and v_l^{n+1} are known after solving Eqs. (20) through (26).

IV. INTERFACIAL CONSTITUTIVE MODELS

The complete set of closure equations is quite lengthy and involves wall shear, a complex wall boiling curve, numerous thermodynamic and transport relations, and the interfacial exchange terms. A detailed discussion of all of these equations is beyond the scope of this paper but an abbreviated description of the interfacial exchange correlations has been included for convenience. The interfacial constitutive equations are basically identical for the one- and three-dimensional portions of TRAC-PF1. A generic description of these relations will be given, and any differences between the one- and three-dimensional models will be noted. The interfacial heat transfer during boiling and the interfacial shear are calculated in conjunction with a simple flow-regime map.⁶ This flow-regime map, although originally developed for vertical pipe flow, is the simplest prescription for defining the constitutive equations by a rational means.

If the void fraction is less than or equal to 0.3 (or $\alpha < 0.5$ if $G > 2700 \text{ kg/m}^2\text{s}$), a bubbly flow is assumed. The interfacial surface area in this regime is calculated in conjunction with a critical bubble Weber number We_b . A value of $We_b = 7.5$ is used in the present code version. This value was chosen based on comparisons between the TRAC predictions and the experimental results for low subcooling (that is, shear-dominated) downcomer tests performed by Creare, Inc. The expression relating interfacial surface area to We_b is

$$\frac{\rho_l V_r^2 D_b}{\sigma} = We_b$$

or

$$D_b = \frac{We_b \sigma}{\rho_l V_r^2} \quad (37)$$

where D_b is the bubble diameter. The bubble diameter must lie between the mesh-cell hydraulic diameter and 10^{-3} m. For this diameter, and assuming a uniform bubble distribution within the mesh-cell volume (vol), the number of bubbles is

$$CNB = \frac{6\pi \text{vol}}{\pi D_b^3} \quad (38)$$

and the interfacial area is

$$A_I = 6\pi \text{vol} \rho_l \frac{V_r^2}{We_b \sigma} \quad (39)$$

If the relative velocity is very small, this area can become small enough to allow significant nonequilibrium. Another surface area,

$$A = 4.83\pi^{2/3} (N_B)^{1/3} \text{vol} \quad (40)$$

based on a minimum number density ($N_B = 10^{10}$ bubbles/m³), is computed and the actual surface area used is the larger of the two.

The liquid-side interfacial heat-transfer coefficient is the larger of an approximate formulation of the Plesset-Zwick bubble growth model,⁸

$$Nu = \frac{1.2}{\pi} (T_\ell - T_B) \rho_\ell \left[\frac{3\rho_\ell}{\rho_g} \frac{\partial T_\ell}{\partial t} + \rho_g (h_{u,g} - h_{u,\ell}) \right] \quad (41)$$

and a sphere convection coefficient,⁹

$$Nu = 2.0 + 0.74 Re_b^{0.5} \quad , \quad (42)$$

where

$$Re_b = \rho_l V_r \frac{D_b}{\mu_l} \quad .$$

The interfacial shear coefficient is provided by a standard set of formulae for a sphere,¹⁰

$$c_l = \frac{3c_h \alpha \rho_l}{4D_b} \quad , \quad (43)$$

where

$$c_h = 240 \text{ for } Re_b < 0.1 \quad ,$$

$$= \frac{24}{Re_b} \text{ for } 0.1 \leq Re_b \leq 2 \quad ,$$

or

$$= \frac{18.7}{Re_b^{0.68}} \text{ for } Re_b > 2 \quad .$$

If the cell-average mass flux is less than $2000 \text{ kg/m}^2\text{s}$ and the vapor fraction is between 0.3 and 0.5, the flow enters the slug regime. At the maximum α of 0.5, 40% of the vapor is assumed to exist in the form of trailing bubbles with the remainder contained in the slug. These bubbles probably contribute to the majority of the interfacial heat transfer and the liquid-side coefficient is calculated from the heat-transfer relations for the entrained bubbles. If the mass flux is greater than $2700 \text{ kg/m}^2\text{s}$, all of the vapor is assumed to exist in bubbly form. Linear interpolation in mass flux is used in the range of 2000 to $2700 \text{ kg/m}^2\text{s}$. In the slug regime the bubble diameter is determined by a linear weighting in α between the Weber number criterion and the channel hydraulic diameter such that the value is the hydraulic diameter at a void fraction of 0.5 and the Weber number size at an α of 0.3.

In the vapor-fraction range of 0.75 to 1.0, an annular or annular-mist regime is assumed. A simple s-shaped entrainment correlation based on the critical Weber number is used. Thus,

$$E = 1 - \exp [(-v_g - v_E) 0.23] , \quad (44)$$

where

$$v_E = 2.3 \left[\frac{(\rho_l - \rho_g) \sigma We_d}{\rho_g^2} \right]^{1/4} .$$

This appears to provide reasonable results for the FLECHT reflood tests. The remainder of the liquid is in a film or sheet. The interfacial shear and heat transfer are volume averages of the film and droplet relations in the annular-mist regime. The wetted surface area of the mesh cell is determined from the rod or slab heat-transfer area in the cell and the portion of the geometric flow area that is blocked off. If the cell is in a region devoid of any structure, the geometric surface area is used as a scaling factor. This, of course, is artificial but in a realistic PWR simulation very few, if any, of the mesh cells are completely free of metal structure. The total interfacial surface area is determined by the sum of the areas contained in the wetted film and the droplets. A critical Weber number equal to 4 for the drops is used with a calculation procedure similar to that for bubbly flow. This value of the Weber number is appropriate for accelerating drops. For those cases where sensitivity to We_d was tested, the results were not influenced strongly by We_d in the range of $2 \leq We_d \leq 12$. The liquid-side heat-transfer coefficient is simply

$$h_{fl} = \frac{ck_l}{D_d} , \quad (45)$$

where c , a constant, has been adjusted to drive the drops to equilibrium under a variety of flow conditions. In the present code, $c = 11300$, which implies a thermal boundary layer in the drops that is about a thousandth of the drop diameter. In the film, a correlation

$$Nu = 0.02 Re \quad (46)$$

is employed to predict h_{fl} . The Dukler annular flow model¹¹ determines the shear for a wavy film, whereas the same drag correlations used for a bubble

are employed if droplets exist. The Dukler model has a gas Reynold's number dependence and is of the form

$$\frac{1}{f_1} = C_1 \log\left(\frac{D}{S} Re_g\right) + C_2 \quad . \quad (47)$$

From the graphical data reported in Ref. 11, we obtain

$$\begin{aligned} C_1 &= 3.04 \text{ and } C_2 = -16.16 \text{ in countercurrent flow and} \\ C_1 &= 5.73 \text{ and } C_2 = -40.61 \text{ in cocurrent flow.} \end{aligned}$$

To avoid the discontinuity that occurs as Re_g becomes small (the correlation is for turbulent flow anyway), smoothing is employed in a transition region. The droplet Reynolds number is defined as

$$Re_d = \frac{\rho_g V_{rd} D_d}{\mu_g} \quad . \quad (48)$$

Because the actual relative velocity calculated is based on a shear that has been averaged between the film and drop correlations, a separate function¹² is used for V_{rd} ,

$$V_{rd} = 2.33 \left[\frac{(\rho_l - \rho_g) \sigma We_b}{\rho_l^2} \right]^{1/4} \quad . \quad (49)$$

For the regime between droplet and bubbly-slug flow, a linear interpolation in the vapor fraction is made between the conditions that would exist if the vapor fraction were at 0.75 in the annular or annular-mist topology and the conditions that would exist if the flow were in the bubbly-slug regime at a void fraction of 0.5. This assures that the correlation for the interfacial shear, interfacial heat transfer, and surface area is a continuous function of the vapor fraction, the relative velocity, the mass flux, and the various fluid thermodynamic and transport properties.

An interface sharpener is used in the lower plenum and core of the three-dimensional vessel to improve the liquid distribution during reflood. Simple void fraction tests are employed to sense the presence of a sharp mixture density discontinuity. The entrainment model then is used to predict the void fraction to be used for convection out of the mesh cell's positive face. This void fraction will always be greater than or equal to the actual void fraction in the cell. The interfacial shear constitutive

relations are calculated based on this void fraction and the scalar field equations use this new value in the z-direction convective terms. A cubic spline is used to merge the sharpened α as the mesh cell fills.

We now discuss the vapor-side heat-transfer coefficient and the liquid heat-transfer coefficient during condensation. The vapor heat-transfer coefficient is a constant, $h_{1g} = 1 \times 10^4$. This implies that the rate for boiling or condensation is determined mainly by the liquid-side coefficient with a vapor coefficient designed to drive the vapor toward the saturation temperature. The formulation for the total liquid heat-transfer coefficient during condensation is based on the following model. If a pipe enters a given three-dimensional mesh cell and the liquid flows into that cell, then a jet is assumed with an α -weighted diameter, a surface area for condensation based on a right circular cylinder is provided, and h_{1l} is given by Eq. (45). If the jet model is not activated, the surface area is the horizontal projected mesh-cell area if $\alpha < 0.5$. The h_{1l} again is given by Eq. (45). In the void region from 0.75 to 1, the same correlations are used for both boiling and condensation (area and h_{1l}). A cubic interpolation connects the regions $0.5 < \alpha < 0.75$.

If the noncondensable gas is present, the condensation rate is reduced according to the prescription

$$\frac{h_{nc}}{h_{1l}} = 0.168 \left[\frac{\sigma \rho_s^2}{\rho_a (1-\alpha) \rho_l} \right]^{0.1}, \quad (50)$$

where h_{nc} is the liquid interfacial heat transfer coefficient with noncondensable gas present. Small cutoffs on $(1-\alpha)$ and ρ_s prevent the denominator from ever becoming close enough to zero to cause difficulties. This model is based on Russian jet data from Ref. 13 and can dramatically reduce condensation when a vapor other than steam is in a region.

If hot metal surfaces are present in a region, then the flashing rate is modified to include the effects of subcooled boiling. If rods or slabs exist and $T_w > T_{sat}$, the h_{wl} is compared to the Dittus-Boelter liquid convective coefficient. If h_{wl} is larger, the difference in wall flux (q_{sb}) is attributed to subcooled boiling and

$$\Gamma = \frac{q_{1l} + q_{1g} + q_{sb}}{h_{lg}}.$$

In both the vapor continuity equation and the vapor thermal-energy equation, the potentials $(T_v - T_g)$ and $(T_g - T_l)$ are evaluated at the new time level, whereas $h_{1g} A_l$ and $h_{1l} A_l$ are evaluated at the old time.

In TRAC-PF1 the one-dimensional components have an additional flow regime if the angle from the horizontal is less than 30° . A stratification criterion based on a modified Froude number analysis developed by A.

Dukler¹⁴ is used to determine if the flow is stratified. The critical velocity U_{crit} is calculated as

$$U_{crit} = C_2 \left[\frac{(\rho_L - \rho_g) g \cos \beta A_g}{\rho_g dA_L/dh_L} \right]^{1/2} \quad (51)$$

$$C_2 = 1 - \frac{h_L}{D}$$

$$\frac{dA_L}{dh_L} = \{D^2 - (2h_L - D)^2\}^{1/2},$$

where h_L is the collapsed liquid height (determined by a standard mensuration formula) and D is the pipe inside diameter. If the absolute value of the vapor velocity is above U_{crit} , the standard flow map is employed. As the vapor velocity goes to zero, the interfacial and wall shear coefficients are calculated by the Blasius relation (but based on a minimum turbulent Reynold's number). A cubic spline employing the independent variable $\ln(V_g)$ connects the two endpoints. This form of interpolation is necessary to prevent oscillations in flow pattern with the large time steps often employed by the code.

In addition, the hydraulic approximation for the difference in gravitational head due to collapsed liquid height variations is added explicitly into the liquid equation of motion. Because this calculation is explicit, horizontal monometer oscillations can occur at larger time step sizes. To prevent this difficulty, the magnitude of this added term is reduced as the time step size is increased. This eliminates the spurious oscillations from occurring.

V. CONCLUSIONS

Although TRAC-PD2 is capable of simulating adequately a wide range of small-break LOCAs, TRAC-PF1 was specifically designed to calculate such accident scenarios quite efficiently, and its use is recommended. Calculations at Los Alamos using this code to model TMI with 80 spatial nodes have been run using 6 min of CDC-7600 computer time for each hour of accident time. In addition to its high computation speed for such transients, PF1 retains the capabilities of previous TRAC versions to calculate all phases of a large-break LOCA and to model multidimensional effects in the vessel region. This makes TRAC-PF1 unquestionably the most versatile computer code available for the analysis of transients in pressurized water reactors.

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